EPA Advanced KM TEQ Calculator

General Instructions: Password to protect/unprotect worksheets = "dioxin"

These instructions apply to this Advanced Kaplan-Meier (KM) Toxicity Equivalent (TEQ) calculator, which includes calculations that support **simple, quasi-sensitivity analysis** that examines the effect of various ways of handling nondetected (ND) or rejected (R-flagged) analytical data results within a sample's congener profile. A Basic version of this calculator is also available for TEQ analyses uncomplicated by high-TEF non-detected congeners or rejected data. The Basic version is also structured to assist TEQ analysis for incremental samples.

BE AWARE

Individual statisticians vary in their acceptance of Helsel's adaptation of the Kaplan-Meier (KM) technique to estimate sample TEQs when nondetected congeners are present. (More details of this technique are covered in the "ND&R discussion" worksheet.) Other methods to avoid simple substitution for nondetects were suggested by peer reviewers of this calculator, and they may be incorporated into future updates of this calculator. The user is advised to seek input from a qualified statistician if important project or site decisions are dependent upon the choice of TEQ calculation method.

Helsel, D.R. 2009. "Summing Nondetects: Incorporating Low-Level Contaminants in Risk Assessment." *Integrated Environmental Assessment and Management.* Volume 6, Number 3. Pages 361 through 366.

The quasi-sensitivity analysis is performed by calculating the TEQ in various ways to estimate the consequences of using or not using ND or rejected (R) data values.
This workbook records TEQs calculated using substitution methods for NDs (0, 1/2-DL, and DL) and the KM method. It also records when R data are used at face value to assess whether the rejected congeners have a significant effect on the reported TEQ. This helps determine whether reanalysis of the sample is necessary. See discussion of ND and R data on the "ND&R discussion" worksheet.

The workbook uses an automated macro that performs the calculations and provides error messages if necessary, allowing the user to correct and repeat the process until the data are correctly entered.

Inserting more sample rows

The "Data entry & SensAnaly-site data" worksheet is set up to accommodate 50 samples. If more than 50 samples are required, samples can be added by unprotecting the worksheet (password is "dioxin") and then adding the needed rows above the last sample rows. The five rows that are associated with an existing sample should be copied onto the new rows. Rows can also be deleted if desired, but it is preferable to leave the data fields blank (including the sample ID in column B). Any blank rows should be inserted above the last sample row at the bottom of the worksheet. If more triplicate rows are necessary, the rows at the top of the template can be copied over other sample rows, or at the end (be sure to insert 15 new rows before doing this). Again, the worksheet will need to be unprotected first. Note that when inserting, deleting or copying rows, it is possible to create program errors, so avoid this if possible.

Excel format

Note that the calculator workbook is saved in Excel 97-2003 Workbook format (*.xls). The workbook should work properly in Excel 2007 and Excel 2010, and may be saved in Excel Macro-Enabled Workbook format (*.xlsm). In Excel 2007 and 2010 versions, the Excel Workbook format (*.xlsx) will not allow the macros in the calculator to operate properly, and should not be used to save the workbook unless all data processing is complete.

Unprotect worksheet

To make some changes to worksheets, the user will need to unprotect the worksheet. Unprotecting the sheet can be performed using the Home/Format/Protection/Unprotect Sheet option. The password is "dioxin". The protection will be re-enabled automatically each time the macro is run, so it is not necessary for the user to manually reenable protection.

Instructions for Macro Use:

Step	Instruction
Enable Macros	Note: Prior to their use, macros will first need to be enabled. In Excel 2007, this can be performed by selecting 'Options' on the Security Warning bar that appears below the Excel menu bars when the workbook is opened, and selecting the 'Enable this content' button, then selecting the 'OK' button. For other versions of Excel, consult Excel HELP to determine how to enable macros. Once macros are enabled, follow the steps below.
1 Hide Columns	Enter the sample numbers in column B of the "Data entry&SensAnaly-site data" worksheet. The sample numbers should be entered in the top row (Row A) of each five-row grouping. If a sample number in any Row A is left blank, the macro will stop operation after the previous sample and will not execute for any samples after this blank sample number. If data are not present for all congeners, the user may leave these columns blank and may hide columns without data. As with deleting and adding rows, the user will have to unprotect the worksheet to hide or unhide columns. Columns should not be deleted from the worksheet. Hide columns using the "Home" me Format/Visibility/Hide & Unhide/Hide Columns.
2 Reorder congeners to match lab report	**Note:** This step is optional, but may help increase the speed and accuracy of manual data input. Check the order of the chemical names to ensure they are listed in the same order as the source data reports that will be used for data input. If they are not in the same order, change numbers in row 6 so that they correspond to the order on the project data reports. Then, click the button labeled "Sort Chemicals", which will run a macro to sort the analytes into the order specified in row 6. Note that the "Congener Abbreviations" worksheet contains a table listing the IUPAC names, CAS numbers, and common abbreviations. This worksheet may be useful in matching the analyte names on the data reports to those in the data entry worksheet. After the sort is complete, check the order of the chemicals again to ensure they are listed in the correct order. This step can be repeated as many times as necessary.
3 EMPC qualifier	Enter the congener data into Row A for each sample, along with qualifiers assigned to each result after the numeric value, if necessary. Valid qualifiers include: • J, E, or A: indicates the sample result for the congener is estimated. • U or ND: indicates the congener was not detected in the sample. • R: indicates the sample result for the congener was rejected. Results flagged as "UJ" should be entered with a "U" qualifier. These are the only qualifiers that should be used. It is not necessary to enter a space between the number and qualifier, but entering a space is also acceptable if the user prefers that approach. If the user wishes to copy and paste data into the spreadsheet, the Paste Values option should be used. To paste values, select "Paste" on the Excel ribbon, then "Paste Special", then "Paste As Values". Note that Row B will be automatically populated by the macro. The user does not need to enter data on this row. Note that if estimated maximum possible concentration (EMPC) values are present, these values should be entered as nondetects (U or ND) with the EMPC value as the detection limit. This will ensure that these values are subjected to the full sensitivity analysis as nondetects with a maximum value of the EMPC. Also see the EMPC discussion in the "ND&R discussion" worksheet.

4
"Donor" values
	Run the macros by clicking on the box labeled "Calculate TEQs" (see cells R1 through T1 of the worksheet "Data entry&SensAnaly-site data"), and then examine Row D for each sample. If there are any samples with congeners that are outlined with a border, these are results for which the user will have the option to enter substitute ("donor") values from a comparable sample; follow the instructions below. If there are no samples with congeners outlined with a border, continue with step 6.
	
	• Values should not be entered for any cell that is not outlined with a border. The outlined cells will fall into two categories. One category is a ND result that is the highest toxic equivalent concentration (TEC) in the sample. The other is a rejected result.
	• Two options are available; option 2 is preferred over option 1. Option 1 should only be used if option 2 is not possible because an analytical result for that congener from another sample cannot be **defensibly substituted**
	  • OPTION 1:
	  - Enter the same value from Row B into the boxed cell in Row D.
	  - Enter "not possible" in column BC, Row C for the sample.
	  • OPTION 2:
	  - Examine the rest of the data set and look for samples with a congener profile and concentrations very similar to the sample in question.
	  - Confirm that the problem congener is detected in that sample. If so, evaluate whether a substitution of the detected value from that sample (a "donor" sample) can defensibly be made for the U/ND. If there is more than one value that could be substituted for the U/ND, use the most conservative (i.e., highest) value. Note that the detected value should be less than or equ to the ND value.
	  - If there is a value from another sample that can be substituted defensibly, enter that value in the boxed cell in Row D.
	  - If there are no values from other samples that can be substituted defensibly **OR** the user prefers to not use substituted ("donor") values, enter the same value from the Row B into the cell outlined with a border in Row D
	Repeat the substitution process for any other congeners in this sample that are outlined with a border, but **DO NOT** select substitute ("donor") values from more than 1 sample for each specific sample.
	
	In column BC, Row C for the sample, enter the sample ID used for substitute ("donor") values for this sample. Note that this is not necessary if Option 1 above was selected, since in this case, the "donor" value comes from the same sample. However, it will be required if Option 2 is used.
	Repeat the congener substitution substeps of Step 4 for all samples.

5	Click on the box labeled "Calculate TEQs" (see cells R1 through T1 of the worksheet "Data entry&SensAnaly-site data"). This will initiate a macro that will copy the entered data to the "KM congener intermediate" worksheet and display the returned results.
6	If any error messages are displayed to the user, examine column AM to see which samples have data entry errors, and correct them (see instructions 1 through 4).
7 "Select KM TEQ" box "Locked" feature Rejected Data	The macro will automatically populate the method for calculating the KM TEQ in column AM "Select KM TEQ" in the uppermost gray cell. As a default, the method that provides the highest KM TEQ will be selected. The user may override this selection and choose another method for calculating the KM TEQ. When the user chooses another method for calculating the KM TEQ in column AM for a sample, the following will be automatically updated: the sample KM TEQ and the qualifiers in columns AJ, AK, and AL. There is another gray box directly below the gray KM TEQ selection box discussed above. Here the user has the option to select **"Locked"**, or leave the cell blank (i.e., unlocked). If "Locked" is selected, the selected KM TEQ option will not be changed when the macro is run again. This can be useful if the user wants to process a few samples at a time, but not lose their selected options for previously processed data. Unlocking: although a blank cell cannot be selected by the drop-down box, the "Locked" option can be removed by deleting the cell contents with the keyboard's DELETE button. If no rejected data are present and no samples have a non-detect for the highest TEC, the macro will select "Section 1" in column AM for all samples. If no rejected data are present and a sample does have a non-detect for the highest TEC, the macro will select either "Section 2 Treatment 1" or "Section 2 Treatment 2" in column AM, whichever is most conservative (highest KM TEQ). The other treatment should be selected if appropriate and justified (for example, if Section 2 Treatment 1 is selected by the macro, the user may select Section 2 Treatment 2 if it is appropriate and justified). If rejected data are present, the macro will select "Section 3" followed by "Treatment 1", "Treatment 2", Treatment 3", or "Treatment 4" in column AM, whichever is most conservative (highest KM TEQ). The most appropriate and justified TEQ should be selected, using the following considerations: The results of the different treatments for handling "R" data should be compared to the decision threshold or used to calculate risk using appropriate risk assessment methods. If the choice of treatment (from more to less conservative) significantly changes the decision outcome, sample reanalysis should be considered. To avoid repeated generation of R-flagged data, ask the laboratory to take corrective action in the reanalysis. An alternative to sample reanalyses is to select a TEQ from the sensitivity analysis for which a transparent, defensible argument can be provided. Note that the result for the TEQs from Substitution in column AG (where NDs are counted as zero) should be the same as the Total TEQ value that is reported on Contract Laboratory Program (CLP) forms (I-HR-CDD-2).
Note 1 Qualifiers	Note regarding sample qualifiers for KM TEQ results: All KM calculations include a determination of the TEC contribution to the TEQ from congener results that are qualified as non-detect, estimated or rejected. If the contribution of these "qualified" TECs to the TEQ is greater than 50 percent, the KM TEQ result should be qualified. The qualifier is determined by the macro, and is shown in a cell in the appropriate Section and Treatment(s), along with the fraction of the TEQ from "qualified" TECs.
Note 2 Adjust TEFs	Note regarding toxic equivalence factors (TEF): The TEFs used in the calculator are from the World Health Organization (WHO) 2005 report. If necessary, the user can change the TEF values to earlier values, or updated values if they are available. The TEFs can also be adjusted for additional sensitivity analysis if desired. To update the TEFs, the user should unprotect the workbook, change the TEFs of concern and then rerun the macro.
Note 3	Note regarding number of detected congeners: There must be at least 3 detected congeners for the methodology in the KM TEQ calculator to be meaningful. If fewer than three detected congeners are present in the results for a sample entered into the calculator, an error message will be displayed to the user. No KM TEQ calculations will be conducted for that sample. "Not calculated" will be displayed in column AN, and a note will be displayed in column AZ stating that fewer than three detected results were present. For discussion, refer to the worksheet "ND&R discussion" under "Treatment of Nondetected Congeners."
Note 4 D/F vs PCB contributions to TEQ	Note regarding dioxin/furan contributions to sample TEQ: In column AN, "Dioxin/Furan" on the third line for each sample refers to the percentage of TEQ contributed from dioxins and furans (this is reported in column AO). The remaining percentage is contributed from dioxin-like PCBs.

For questions about this Calculator, contact Deana Crumbling at USEPA, crumbling.deana@epa.gov or (703) 603-0643.

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EPA Advanced KM TEQ Calculator

This material is reproduced from the discussion (27Sep10 version) presented in Appendix 4 of the dioxi

Appendix 4: Calculation of Total Dioxin TEQs with Nondetect and Rejected Congeners

Helsel's Kaplan-Meier Approach

Calculation of sums or totals for multi-constituent chemicals [e.g., total dioxin TEQs, total PCBs, total polycyclic aromatic hydrocarbons (PAHs), etc.] has typically involved simple substitution of zero, one-half the detection limit (DL), or the DL for left-censored (nondetect or less-than values) congeners. Because this practice introduces bias to estimates used in statistical calculations, however, many sources now strongly recommend against the use of arbitrary surrogate values for nondetects (Helsel 1990, 2005a, 2005b, 2009; EPA 2006, 2009a, 2009b).

Helsel (2009) describes an approach for calculating totals using the KM product limit estimator, which is based on the following relationship between the "mean" of the toxic equivalence concentrations (TECs) and total TEQ for samples containing multiple congeners:

total concentration = "mean" TEC x n (where n is the number of congeners)

Note that this "mean" TEC is an intermediate value in the calculation that has no relationship to a mean TEQ for replicate DU samples. The KM estimator is a nonparametric maximum likelihood estimator that has been widely used in survival and failure analysis for more than 50 years (Kaplan and Meier 1958, Klein and Moeschberger 2003, Meeker and Escobar 1998). The KM estimator has only recently come into use in environmental assessment studies (Helsel 2005a), and is currently a default method used in EPA's ProUCL software for calculating the 95% UCL of the mean for data with one or more censored results (EPA 2009a, 2009b).

Treatment of Nondetected Congeners

For the purposes of this dioxin reassessment UFP-QAPP template, the intermediate KM "mean" is recommended for use in calculating total dioxin TEQs, using the general equation presented above, in all cases where a) some fraction of the congeners are nondetect, and b) there are at least three detected congeners. Additional guidelines for calculating the KM intermediate "mean" are provided below. If all congeners are detected, then the intermediate "mean" calculated by the equation is the arithmetic average of all the congeners' TECs.

If only one or two congeners are detected, then there is no statistically satisfactory method for calculating the dioxin TEQ that adequately accounts for the uncertainty introduced by nondetect congener results. In this case, the intermediate "mean" should be calculated as the arithmetical average, where simple substitution is used for nondetects. A quasi-sensitivity analysis approach is recommended, wherein substitution of both zero and the DL are used to calculate lower- and upper-bound estimates for the total TEQ. Compare the

recommended. Cases where only one or two congeners are detected are discussed above. Lastly, Helsel (2009) recommends that for left-censored environmental data, Efron's bias correction should always be used. This simply requires that the minimum result always be treated as a detected result. The manner in which Efron's bias correction is incorporated in calculations of the KM mean depends on the specific software or approach used. For example, for programs that require a "flag" to distinguish between detected and nondetect data, one only needs to use the appropriate flag for detected data to qualify the minimum result(s).

Three options are described below for calculation of the KM mean:

(1) Helsel's KM Excel spreadsheet model (available from www.practicalstats.com). This spreadsheet has been built into a workbook designed specifically for calculating the TEQ from raw data congener concentration data. Raw data are entered into one spreadsheet, which automatically calculates the toxic equivalent concentration (TEC) for each congener. The TECs are copied and pasted into a second spreadsheet in the workbook that performs the KM calculation. This produces an intermediate value (the KM "mean") which is transferred back to the first spreadsheet. The intermediate result is then automatically multiplied by the number of congeners to produce the total TEQ for the sample. Detailed instructions for using the spreadsheets are included in the Excel workbook's spreadsheets.

(2) Alternatively, EPA's ProUCL software may be used. Before estimates of the KM intermediate "mean" TEC can be calculated, the congener concentration results (in ppt) must be converted to congener TECs by multiplying each congener by its TEF. This must be done independently before the TECs are put into ProUCL for the KM calculation. (ProUCL cannot do the TEC calculation.) The TECs are then entered into ProUCL and the KM intermediate "mean" is automatically calculated for data sets with one or more nondetect results. EPA (2009a, 2009b) should be consulted for instructions for entering data into ProUCL, since a coding procedure must be used in ProUCL to "tell it" which congener TECs were from ND values. Note that in order to use Efron's bias correction, the minimum result should be coded as a detected result. If intermediate "means" are required for multiple samples, then each sample needs to be identified using a "grouping" variable (see EPA 2009a). For each sample, the KM intermediate "mean" will need to be extracted from the ProUCL report, and manually multiplied by the number of congeners to produce the total TEQ result for that sample.

(3) Commercial or other statistical software. The KM model is included in many mainstream statistical software packages, as well as public domain (including the R language) programs. Helsel (2005a) discusses an approach for "flipping" data for use in commercial packages, which emphasize treatment of right-censored data. Experienced users may elect to use alternative approaches for calculation of the KM intermediate "mean," but must use methods employing Efron's bias correction, and must demonstrate that results are comparable to the intermediate "means" calculated using Options (1) or (2) above.

elect to perform a quasi-sensitivity analysis by calculating TEQ without the EMPC values. As for rejected data, significant effects from EMPC values may require corrective action to improve data quality (such as sample reanalysis).

Therefore, for congeners that are influential (high-toxicity, TEF close to 1, or high concentration) in calculations of the intermediate "mean" and total TEQ, rejected and qualified data may require further evaluation by project teams. The uncertainty of calculating total TEQs, as can be demonstrated through sensitivity analyses, should be addressed in the uncertainty section of assessment documents, and taken into account in decision making.

in reassesment UFP-QAPP User Guide.

TEQs from both approaches to assess whether they have the same decision outcome. Substitution of one-half the DL can be used to calculate a "middle-of-the-road" value, although it should be acknowledged that the uncertainty of this estimate may be unacceptable for decision making.

In cases where critical decisions hinge on total TEQ estimates with mostly nondetect results, project teams are advised to consider

- consulting personnel with expertise in statistics,
- reanalyzing existing samples (if archived samples are available and meet holding times),
- comparing with results from nearby similar DUs and the CSM, or
- collecting additional samples.

The stepwise KM approach for calculating the total dioxin TEQ for individual samples is described below:

Step 1. Calculate the TEC for each congener by multiplying the results for individual congeners by their congener-specific TEF (van den Berg and others 2006). For nondetect congeners, the reporting limit or DL should be multiplied by the TEF.

Step 2. Calculate the intermediate "mean" TEC for each sample using a KM calculator spreadsheet. If all the congeners are detected, then calculate the intermediate value as the arithmetic mean. If nondetects are present and at least three results are detected, calculate the KM intermediate using one of the options described below. If only one or two congeners are detected, use simple substitution and a quasi-sensitivity analysis approach, as discussed above.

Step 3. Calculate the total dioxin TEQ using: Total TEQ = intermediate "mean" TEC x n, where n is the number of congeners in the calculation.

Helsel (2009) discusses several potential contraindications for calculation of the KM mean. The first concerns cases where only a single DL is used for all nondetect congeners. This is not expected to occur for calculation of total dioxin TEQs, since results for individual congers are first multiplied by congener-specific TEFs. The second contraindication is when the maximum reported result is a nondetect, high-toxicity (i.e., TEF close to 1) congener. This is problematic, as the KM method will effectively ignore maximum results that are censored. Helsel (2009) suggests that the DL be substituted in these cases, but that it should be acknowledged that this represents a worst-case scenario. Another option is to compare the congener concentration and congener profile of the sample with a high TEF nondetect to results from similar (per the CSM) DUs. If the congener profiles are similar, but the other DUs have a detection for the congener in question, substitution of a value (straight substitution, an average of several, or a maximum) from the other DUs may be made.

Helsel (2009) does not discuss the minimum number of detected results required to estimate the KM mean, but a practical minimum of three detected results is

Treatment of R-Qualified Congeners

One additional component for assessing the uncertainty of estimates of the intermediate KM "mean" and total TEQ, concerns treatment of rejected (R qualified) data. It is possible to reject individual congener analytes based on ion abundance, the signal-to-noise ratio, relative retention time, a low laboratory control sample result, gross blank contamination, or other analyte-specific criteria. For non-dioxin individual chemicals with multiple-sample sample sets (i.e., sufficient sample-sizes to support calculations), rejected data are always excluded from calculations in environmental assessments. However, for calculation of the "mean" (and total) for a set of congeners, there is concern that exclusion of rejected data may bias estimates low or create a need for replacement data (resampling or reanalysis). The magnitude (and importance) of this bias will of course depend on the values reported for R-qualified data, as well as the congener-specific TEFs.

Although rejected data should not be included in final calculations of TEQ for a given sampling or decision unit, rejected data values (concentrations or detection limits) can be included in KM "mean" and total TEQ calculations early in the data evaluation process. These TEQs can be compared to TEQs calculated with the rejected values removed. This quasi-sensitivity approach, similar to that recommended above for nondetect values, will assist project teams in assessing the magnitude of impacts from rejected data and the need for replacement data (Replacement data may require reanalysis of samples at the laboratory, with laboratory corrective actions or method refinements as needed, or the collection of additional samples from the site). Rejected data can be further evaluated through professional judgment, such as whether a rejected congener may be present at a concentration that could affect the TEQ based on historical site information or data from surrounding decision units. For example, project teams could use the KM calculator to further assess how high the concentration of a rejected congener would have to be to affect the TEQ, and then compare this estimate to concentrations for this congener that are present in other decision units, or in comparable historical data sets.

Treatment of EMPC values and qualified data

The CLP SOW for dioxin analysis specifies the reporting of detected congeners as "EMPC" values ("estimated maximum possible concentration") when a congener peak is present at an acceptable signal-to-noise ratio, but ion abundance criteria are not met for definitive identification of that congener. The CLP SOW excludes these values from the calculation of TEQ. EPA Method 8290A also specifies the reporting of EMPC values but makes no recommendations concerning their use in TEQ calculations. EMPC values are generally qualified as estimated concentrations ("J") or nondetect values ("U") during data validation in accordance with EPA Functional Guidelines. When qualified "J", EMPC values can be applied along with other J-qualified congener results in TEQ calculation and risk assessment (J-qualified data are generally applied like unqualified data under EPA risk assessment protocols). EMPC values qualified "U" can be treated as other nondetect values using the KM approach described above. Given that use of EMPC values may overestimate the TEQ and associated dioxin risk, project teams may again

References

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EPA Advanced KM TEQ Calculator

Advanced KM TEQ calculator for performing quasi-sensitivity analyses

Project Name:
Matrix:
Units:
Data entered by:
Date entered:

protect/unprotect sheet password = dioxin

SITE DATA

Chemical Sort Order:	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29
WHO 2005 TEFs =	**1**	**1**	**0.1**	**0.1**	**0.1**	**0.01**	**0.0003**	**0.1**	**0.03**	**0.3**	**0.1**	**0.1**	**0.1**	**0.1**	**0.01**	**0.01**	**0.0003**	**0.0001**	**0.0003**	**0.00003**	**0.00003**	**0.00003**	**0.00003**	**0.1**	**0.00003**	**0.00003**	**0.00003**	**0.03**	**0.00003**
Sample ID: **(must enter on Row A)**	**TCDD**	**PeCDD**	**1,4-HxCDD**	**1,6-HxCDD**	**1,9-HxCDD**	**1,4,6-HpCDD**	**OCDD**	**TCDF**	**1-PeCDF**	**4-PeCDF**	**1,4-HxCDF**	**1,6-HxCDF**	**1,9-HxCDF**	**4,6-HxCDF**	**1,4,6-HpCDF**	**1,4,9-HpCDF**	**OCDF**	**PCB 77**	**PCB 81**	**PCB 105**	**PCB 114**	**PCB 118**	**PCB 123**	**PCB 126**	**PCB 156**	**PCB 157**	**PCB 167**	**PCB 169**	**PCB 189**

TEQs from Substitution			KM Method		
U = 0 & sum	U = 1/2 DL & sum	U = DL & sum	Sample KM TEQ	Qualifier	Select KM TEQ

(Quasi) Sensitivity Analysis SECTION 1		(Quasi) Sensitivity Analysis SECTION 2				(Quasi) Sensitivity Analysis SECTION 3										
Highest TEC value is a DETECT, and there are no rejected ("R") values		Highest TEC value is a NONDETECT ("U" or "ND"), and there are no rejected ("R") values				Rejected ("R") value(s) are present; nondetected values ("U" or "ND") may or may not be present, and the highest TEC may or may not be a nondetected result.										
Treatment 1		Treatment 1: Make highest U value a D		Treatment 2: Substitute comparable "donor" value for highest U		Treatment 1: TEQ as simple sum when R & U treated as 0 (minimum)		Treatment 2: TEQ as simple sum when R & U treated as normal detects		Treatment 3: Used if "donor" value is available for R values		Treatment 4: Used if "donor" values are available for R and U values				
KM TEQ	Qualifier and Qualifier Fractions	KM TEQ	Qualifier and Qualifier Fractions	KM TEQ	Qualifier and Qualifier Fractions	KM TEQ	Qualifier and Qualifier Fractions	KM TEQ	Qualifier and Qualifier Fractions	KM TEQ	Qualifier and Qualifier Fractions	KM TEQ	Qualifier and Qualifier Fractions	Will sample reanalysis be requested?	Sample ID used for "donor" values	Comment

Sample notes

value to use: Row B
congener TEC: Row C
donor value to use: Row D
donor TEC: Row E

value to use: Row B
congener TEC: Row C
donor value to use: Row D
donor TEC: Row E

value to use: Row B
congener TEC: Row C
donor value to use: Row D
donor TEC: Row E

value to use: Row B
congener TEC: Row C
donor value to use: Row D
donor TEC: Row E

value to use: Row B
congener TEC: Row C
donor value to use: Row D
donor TEC: Row E

value to use: Row B
congener TEC: Row C
donor value to use: Row D
donor TEC: Row E

value to use: Row B
congener TEC: Row C
donor value to use: Row D
donor TEC: Row E

value to use: Row B
congener TEC: Row C
donor value to use: Row D
donor TEC: Row E

value to use: Row B
congener TEC: Row C
donor value to use: Row D
donor TEC: Row E

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congener TEC: Row C
donor value to use: Row D
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donor TEC: Row E

value to use: Row B
congener TEC: Row C
donor value to use: Row D
donor TEC: Row E

value to use: Row B
congener TEC: Row C

EPA Advanced KM TEQ Calculator

Advanced KM TEQ calculator for performing quasi-sensitivity analyses

Project Name:			
Matrix:		**Data entered by:**	
Units:		**Date entered:**	

protect/unprotect sheet password = dioxin

SITE DATA

Sample notes	Sample ID: (must enter on Row A)	TCDD	PeCDD	1,4-HxCDD	1,6-HxCDD	1,9-HxCDD	1,4,6-HpCDD	OCDD	TCDF	1-PeCDF	4-PeCDF	1,4-HxCDF	1,6-HxCDF	1,9-HxCDF	4,6-HxCDF	1,4,6-HpCDF	1,4,9-HpCDF	OCDF	PCB 77	PCB 81	PCB 105	PCB 114	PCB 118	PCB 123	PCB 126	PCB 156	PCB 157	PCB 167	PCB 169	PCB 189
	Chemical Sort Order:	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29
	WHO 2005 TEFs =	1	1	0.1	0.1	0.1	0.01	0.0003	0.1	0.03	0.3	0.1	0.1	0.1	0.1	0.01	0.01	0.0003	0.0001	0.0003	0.00003	0.00003	0.00003	0.00003	0.1	0.00003	0.00003	0.00003	0.03	0.00003
	donor value to use: Row D donor TEC: Row E																													
	value to use: Row B congener TEC: Row C donor value to use: Row D donor TEC: Row E																													
	value to use: Row B congener TEC: Row C donor value to use: Row D donor TEC: Row E																													
	value to use: Row B congener TEC: Row C donor value to use: Row D donor TEC: Row E																													
	value to use: Row B congener TEC: Row C donor value to use: Row D donor TEC: Row E																													
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	value to use: Row B congener TEC: Row C donor value to use: Row D donor TEC: Row E																													
	value to use: Row B congener TEC: Row C donor value to use: Row D donor TEC: Row E																													

Sample ID	TEQs from Substitution			KM Method			(Quasi) Sensitivity Analysis SECTION 1		(Quasi) Sensitivity Analysis SECTION 2				(Quasi) Sensitivity Analysis SECTION 3										
							Highest TEC value is a DETECT, and there are no rejected ("R") values		Highest TEC value is a NONDETECT ("U" or "ND"), and there are no rejected ("R") values				Rejected ("R") value(s) are present; nondetected values ("U" or "ND") may or may not be present, and the highest TEC may or may not be a nondetected result.										
							Treatment 1		Treatment 1: Make highest U value a D		Treatment 2: Substitute comparable "donor" value for highest U		Treatment 1: TEQ as simple sum when R & U treated as 0 (minimum)		Treatment 2: TEQ as simple sum when R & U treated as normal detects		Treatment 3: Used if "donor" value is available for R values		Treatment 4: Used if "donor" values are available for R and U values				
	U = 0 & sum	U = 1/2 DL & sum	U = DL & sum	Sample KM TEQ	Qualifier	Select KM TEQ	KM TEQ	Qualifier and Qualifier Fractions	KM TEQ	Qualifier and Qualifier Fractions	KM TEQ	Qualifier and Qualifier Fractions	KM TEQ	Qualifier and Qualifier Fractions	KM TEQ	Qualifier and Qualifier Fractions	KM TEQ	Qualifier and Qualifier Fractions	KM TEQ	Qualifier and Qualifier Fractions	Will sample reanalysis be requested?	Sample ID used for "donor" values	Comment
donor value to use: Row D donor TEC: Row E																							
value to use: Row B congener TEC: Row C donor value to use: Row D donor TEC: Row E																							
value to use: Row B congener TEC: Row C donor value to use: Row D donor TEC: Row E																							
value to use: Row B congener TEC: Row C donor value to use: Row D donor TEC: Row E																							
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value to use: Row B congener TEC: Row C donor value to use: Row D donor TEC: Row E																							

DATA LIST

List of TEQ results to copy and paste into other spreadsheets, such as ProUCL

CAUTION: double-check entries and gray cells for anomalous entries

Line	Sample ID	TEQ Result	Qualifier
line #1			
line #2			
line #3			
line #4			
line #5			
line #6			
line #7			
line #8			
line #9			
line #10			
line #11			
line #12			
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line #43			
line #44			
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line #46			
line #47			
line #48			
line #49			
line #50			

EPA Advanced KM TEQ Calculator

KMStats v 1.4 Practical Stats

Input data to the blue cells, then sort from highest to lowest concentration. Concentrations and detection limits in Col A.
Number of detects at each concentration in Col B.
Number of nondetects at each DL in Col C.

For details on the Kaplan-Meier method, see
Helsel, D.R. (2012), **Statistics for Censored Environmental Data Using Minitab and R**, 2nd ed. Wiley and Sons. 324 pp.

protect/unprotect sheet password = dioxin

congener TEC	# Detects	# Nondetects	Quantiles	
		1	0.000	
		1	0.000	
		1	0.000	
		1	0.000	
		1	0.000	
		1	0.000	
		1	0.000	
		1	0.000	
		1	0.000	
		1	0.000	
		1	0.000	
		1	0.000	
		1	0.000	**KM intermediate "mean"**
		1	0.000	0.0000
		1	0.000	
		1	0.000	**KM TEQ**
		1	0.000	0.0000
			0.000	
			0.000	
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			0.000	

		Constant	Flip Conc	rank	ranksum	at risk	partial prob	S	For P50	Max50	Row50	For P25	Max25	Row25	For P75	Max75	Row75	For Mean	Rectangles	DiffC	LagP	Cum Area	Ar	Ar2
0	0	1	0	0	0	0	0	1	0	0	2	0	0	2	0	0	2	0	1	1	1	1	0	0
0	0		0	0	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	1	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	2	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0	#Rows with h	0	3	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0	1	0	4	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0	1	0	5	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0	2	0	6	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	7	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	8	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	9	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	10	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	11	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	12	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	13	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	14	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	15	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
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0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0
0	0		0	16	0	0	0	1	0	0		0	0		0	0		0	0	0	1	0	0	0

Abbreviation 1	Abbreviation 2	IUPAC name	CAS #	Type
TCDD	2,3,7,8-TCDD	2,3,7,8-Tetrachlorodibenzo-p-dioxin	1746-01-6	Dioxin
PeCDD	1,2,3,7,8-PeCDD	1,2,3,7,8-Pentachlorodibenzo-p-dioxin	40321-76-4	Dioxin
1,4-HxCDD	1,2,3,4,7,8-HxCDD	1,2,3,4,7,8-Hexachlorodibenzo-p-dioxin	39227-28-6	Dioxin
1,6-HxCDD	1,2,3,6,7,8-HxCDD	1,2,3,6,7,8-Hexachlorodibenzo-p-dioxin	57653-85-7	Dioxin
1,9-HxCDD	1,2,3,7,8,9-HxCDD	1,2,3,7,8,9-Hexachlorodibenzo-p-dioxin	19408-74-3	Dioxin
1,4,6-HpCDD	1,2,3,4,6,7,8-HpCDD	1,2,3,4,6,7,8-Heptachlorodibenzo-p-dioxin	35822-39-4	Dioxin
OCDD	1,2,3,4,5,6,7,8-OCDD	Octachlorodibenzo-p-dioxin	3268-87-9	Dioxin
TCDF	2,3,7,8-TCDF	2,3,7,8-Tetrachlorodibenzofuran	51207-31-9	Furan
1-PeCDF	1,2,3,7,8-PeCDF	1,2,3,7,8-Pentachlorodibenzofuran	57117-41-6	Furan
4-PeCDF	2,3,4,7,8-PeCDF	2,3,4,7,8-Pentachlorodibenzofuran	57117-31-4	Furan
1,4-HxCDF	1,2,3,4,7,8-HxCDF	1,2,3,4,7,8-Hexachlorodibenzofuran	70648-26-9	Furan
1,6-HxCDF	1,2,3,6,7,8-HxCDF	1,2,3,6,7,8-Hexachlorodibenzofuran	57117-44-9	Furan
1,9-HxCDF	1,2,3,7,8,9-HxCDF	1,2,3,7,8,9-Hexachlorodibenzofuran	72918-21-9	Furan
4,6-HxCDF	2,3,4,6,7,8-HxCDF	2,3,4,6,7,8-Hexachlorodibenzofuran	60851-34-5	Furan
1,4,6-HpCDF	1,2,3,4,6,7,8-HpCDF	1,2,3,4,6,7,8-Heptachlorodibenzofuran	67562-39-4	Furan
1,4,9-HpCDF	1,2,3,4,7,8,9-HpCDF	1,2,3,4,7,8,9-Heptachlorodibenzofuran	55673-89-7	Furan
OCDF	1,2,3,4,5,6,7,8-OCDF	Octachlorodibenzofuran	39001-02-0	Furan
PCB 77	3,3',4,4'-TCB	3,3',4,4'-Tetrachlorobiphenyl	32598-13-3	Dioxin-like PCB
PCB 81	3,4,4',5-TCB	3,4,4',5-Tetrachlorobiphenyl	70362-50-4	Dioxin-like PCB
PCB 105	2,3,3',4,4'-PeCB	2,3,3',4,4'-Pentachlorobiphenyl	32598-14-4	Dioxin-like PCB
PCB 114	2,3,4,4',5-PeCB	2,3,4,4',5-Pentachlorobiphenyl	74472-37-0	Dioxin-like PCB
PCB 118	2,3',4,4',5-PeCB	2,3',4,4',5-Pentachlorobiphenyl	31508-00-6	Dioxin-like PCB
PCB 123	2,3',4,4',5'-PeCB	2,3',4,4',5'-Pentachlorobiphenyl	65510-44-3	Dioxin-like PCB
PCB 126	3,3',4,4',5-PeCB	3,3',4,4',5-Pentachlorobiphenyl	57465-28-8	Dioxin-like PCB
PCB 156	2,3,3',4,4',5-HxCB	2,3,3',4,4',5-Hexachlorobiphenyl	38380-08-4	Dioxin-like PCB
PCB 157	2,3,3',4,4',5'-HxCB	2,3,3',4,4',5'-Hexachlorobiphenyl	69782-90-7	Dioxin-like PCB
PCB 167	2,3',4,4',5,5'-HxCB	2,3',4,4',5,5'-Hexachlorobiphenyl	52663-72-6	Dioxin-like PCB
PCB 169	3,3',4,4',5,5'-HxCB	3,3',4,4',5,5'-Hexachlorobiphenyl	32774-16-6	Dioxin-like PCB
PCB 189	2,3,3',4,4',5,5'-HpCB	2,3,3',4,4',5,5'-Heptachlorobiphenyl	39635-31-9	Dioxin-like PCB

Acronym List	
A	Data qualifier used to indicate an estimated result.
CAS	Chemical abstracts service
CLP	Contract Laboratory Program
CSM	Conceptual site model
CV	Coefficient of variation
DL	Detection limit
DU	Decision unit
E	Data qualifier used to indicate an estimated result.
EMPC	Estimated maximum (protocol) concentration
EPA	U.S. Environmental Protection Agency
HpCDD	Heptachlorodibenzo(p)dioxin
HpCDF	Heptachlorodibenzofuran
HxCDD	Hexachlorodibenzo(p)dioxin
HxCDF	Hexachlorodibenzofuran
ICS	Incremental composite sample
ISM	Incremental sampling methodology
ITRC	Interstate Technology and Regulatory Council
J	Data qualifier used to indicate an estimated result.
KM	Kaplan-Meier
ND	Nondetect
OCDD	Octachlorodibenzo(p)dioxin
OCDF	Octachlorodibenzofuran
PCB	Polychlorinated biphenyl
PeCDD	Pentachlorodibenzo(p)dioxin
PeCDF	Pentachlorodibenzofuran
QC	Quality control
R	Data qualifier used to indicate a rejected result.
RSD	Relative standard deviation
SD	Standard deviation
SOW	Scope of work
TCDD	Tetrachlorodibenzo(p)dioxin
TCDF	Tetrachlorodibenzofuran
TEC	Toxic equivalent concentration
TEF	Toxic equivalence factor
TEQ	Toxic equivalents
U	Data qualifier used to indicate a nondetected result.
UCL	Upper confidence limit
WHO	World Health Organization